

Shift and broadening of resonance lines of antiprotonic helium atoms in solid helium

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Abstract

We have estimated the shift and broadening of the resonance lines in the spectrum of antiprotonic helium atoms $\bar{p}\text{He}^+$ implanted in solid helium ^4He . The application of the response function for crystalline helium has enabled determination of the contributions from the collective degrees of freedom to the shift and broadening. It occurs that the broadening due to the collective motion is negligible compared to the natural line width. The available pair-correlation functions for crystalline ^4He have been applied for estimating the resonance-line shift due to collisions of $\bar{p}\text{He}^+$ atom with the surrounding ^4He atoms. The dependence of the line shift, which has been calculated in the quasistatic limit, on the solid- ^4He density is nonlinear.

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I. INTRODUCTION

The aim of this work is estimation of the shift and broadening of resonance lines of the $\bar{p}\text{He}^+$ atoms in solid ^4He as functions of helium density. A similar study for liquid ^4He , presented in Ref. [1], showed that the shift is a linear function of density in normal-fluid ^4He and displays only small oscillations with temperature in superfluid ^4He . The pair-distribution function, which describes the atom distribution around a given particle, is very similar for both the normal-fluid and the superfluid helium at various temperatures and saturated-vapor pressure. Also, the density change for liquid ^4He at such a pressure is lower than about 15%. Therefore, solid ^4He gives the possibility of studying the resonance-line shift and broadening at much higher densities and thus for shorter distances between the atoms.

The antiprotonic helium atoms are created when antiprotons are decelerated in helium targets and then replace one electron in the helium atoms. About 3% of antiprotons are captured in metastable states (n, ℓ) with long lifetimes on the order of microseconds [2]. This phenomenon enabled high-precision laser spectroscopy of $\bar{p}\text{He}^+$ atoms. As a result, the antiproton-to-electron mass ratio [3] has been determined with the best accuracy up-to-date. Such high-precision measurements required the estimation of different systematic effects. Among the most important effects are the shift and broadening of the spectral lines due to interaction with the helium atoms and varying with the density of the helium target. In the case of helium gas, these effects have been calculated in the semiclassical approach with the use of a pairwise potential of interaction between the $\bar{p}\text{He}^+$ atom and an ordinary helium atom [4]. The calculation results agree well with the experimental data up to the gaseous-helium density $\varrho = 127 \text{ g/l}$ [2]. It has been found that the resonance line shifts in these gas targets are proportional to the helium density within the experimental accuracy [5, 6]. The attempts for laser spectroscopy of antiprotonic helium atoms in liquid helium, which were performed by the ASACUSA Collaboration at CERN [7], encouraged us to evaluate the corresponding shifts and broadening in fluid and superfluid ^4He [1]. In the case of liquid helium, it was necessary to take into account the influence of collective dynamics of helium atoms on the shifts and broadening of spectral lines, apart from the collisional effects. Our calculations were performed for the target temperatures $T = 1.0\text{--}4.27 \text{ K}$ at pressures P up to 8 bars, which corresponds to the maximum pressure applied in the gaseous-helium experiments. For such conditions, the maximum density of about 146 g/l is reached at the λ point. Our calculations confirmed the linear dependence of the resonance-line shift in normal-fluid ^4He . On the other hand, an appreciable oscillation (9%) of this shift as a function of temperature was found for the region of superfluid, where the ^4He density is practically constant.

At the atmospheric pressure, helium remains liquid even at absolute zero, due to the weak interaction between the helium atoms and the large zero-point motion of these atoms. However, the application of pressure $P \approx 25 \text{ bar}$ below a few kelvins leads to solidification of ^4He [8]. The solid helium at the melting line has a density significantly greater than that of liquid helium. The solid- ^4He density can be increased using even larger pressures.

In this work, the numerical calculations are performed for the transition $|i\rangle = (n, \ell) = (39, 35) \rightarrow |f\rangle = (n', \ell') = (38, 34)$ between the initial $|i\rangle$ and final $|f\rangle$ states of the $\bar{p}\text{He}^+$ atom (transition 1), which has been experimentally observed even at a relatively high density of 127 g/l [3]. The resonance wavelength for this transition equals $\lambda_0 = 5972.570 \text{ \AA}$ [5] and the corresponding resonance energy is $E_0 = 2.07589 \text{ eV}$. In the case of this line, the Auger

decay rate $R_A \approx 1.11 \times 10^8 \text{ s}^{-1}$ [9] determines the natural line width Γ_0 , according to the relation

$$\Gamma_0 \approx \hbar R_A, \quad (1)$$

which gives $\Gamma_0 \approx 0.73 \times 10^{-7} \text{ eV}$. The corresponding frequency $\nu_n = \Gamma_0/h$ equals 0.018 GHz.

In Sec. II we estimate the changes of the line profile due to the collective motion in the quantum crystal ^4He , using the method presented in Ref. [10]. The line shift, which is caused by collisions of $\bar{p}\text{He}^+$ atom with neighboring ^4He atoms, is calculated in Sec. III in the quasistatic approximation of Ref. [1] using the available pair-correlation functions $g(r)$ for crystalline ^4He . It has been shown in Ref. [1] that in the quasistatic limit of slow collisions the semiclassical expression for the collisional shift of Ref. [4] takes the form of a mean value of the interatomic potential, averaged over the spatial distribution of the perturbing helium atoms around the emitting antiprotonic atoms. Under the assumption that the latter is close to the distribution in pure helium, described by the pair-correlation function, this allows for using experimental data about $g(r)$. Unfortunately the semiclassical expression for the line broadening [4] does not take any simple form in the quasistatic limit, so that the collisional width remains to be evaluated by full scale semiclassical or quantum calculations, which is beyond the scope of the present Brief Report. The results are briefly discussed in Sec. IV.

II. LINE SHIFT AND BROADENING DUE TO THE COLLECTIVE DYNAMICS OF SOLID HELIUM

The shift and broadening of a resonance line can be evaluated using the method developed by Singwi and Sjölander [10], which employs the Van Hove formalism of the response function [11]. When a particle which absorbs or emits a photon is set at a fixed position, the absorption cross section σ_a takes the following form

$$\sigma_a(E) = \sigma_0 \frac{\Gamma_0^2/4}{(E - E_0)^2 + \Gamma_0^2/4} \quad (2)$$

where E is the photon energy, σ_0 is the resonance maximum at the resonance energy E_0 and Γ_0 stands for the natural width of the resonance. In the case of a harmonic crystal, the resonance profile $\sigma_a^{\text{solid}}(E)$ can be rigorously derived. For a monoatomic cubic Bravais lattice, the exact form of the profile is given as [10]

$$\begin{aligned} \sigma_a^{\text{solid}}(E) = \frac{\pi\sigma_0\Gamma_0}{2} \exp(-2W) & \left[\frac{1}{2\pi} \frac{\Gamma_0}{(E - E'_0)^2 + \frac{1}{4}\Gamma_0^2} \right. \\ & \left. + \sum_{n=1}^{\infty} g_n(\omega, T) \frac{(2W)^n}{n!} \right], \end{aligned} \quad (3)$$

where $\hbar\omega$ and $\hbar q$ denote the energy and momentum transfer to the crystal, respectively, and T is temperature. Although solid ^4He has the hcp structure under specific conditions (see the phase diagram, e.g., in Ref. [8]), apart from the cubic bcc and fcc structures, the above expansion establishes a fair approximation also for this lattice. In the case of laser-stimulated transitions in the antiprotonic helium, the resonance energy in Eq. (3) equals $E'_0 = E_0 + \Delta E_0$, where ΔE_0 is the line shift due to the pairwise interaction. The exponent $2W$ of the Debye-Waller factor $\exp(-2W)$ can be expressed as follows

$$2W = E_r \int_0^\infty \frac{Z(w)}{w} \coth\left(\frac{1}{2}\beta_T w\right) dw, \quad \beta_T = \frac{1}{k_B T}, \quad (4)$$

where $Z(w)$ is the normalized density of vibrational states in the crystal, k_B is Boltzmann's constant and E_r denotes the recoil energy

$$E_r = \frac{(\hbar q)^2}{2M}, \quad (5)$$

in which M is the mass of antiprotonic helium.

The first term in the expansion (3) describes the recoil-less photon absorption or emission in the rigid crystal lattice. The next terms of this expansion, which are proportional to q^{2n} , describe the same process with simultaneous absorption or emission of one or more phonons. The functions g_n from Eq. (3) are defined in Ref. [10]. In particular, the one-phonon term $2Wg_1$ in the brackets of this equation takes the following form

$$2Wg_1(\omega, T) = E_r \frac{Z(\omega)}{\omega} [n_B(\omega, T) + 1], \quad (6)$$

where

$$n_B(\omega, T) = [\exp(\beta_T \omega) - 1]^{-1} \quad (7)$$

is the Bose population factor for phonons. The amplitudes of all the processes are determined by the Debye-Waller factor. When $2W \ll 1$ for a specific photon energy, target and temperature (strong-binding case), the recoil-less term is significant. Such a situation takes place in the case of the Mössbauer effect.

When a photon is absorbed or emitted by the antiprotonic helium atom, the momentum and energy transfers to the crystal lattice are equal to

$$\hbar q = p, \quad \hbar \omega = E - E'_0, \quad (8)$$

respectively. The absolute value of the photon momentum is denoted here by p . In the case of transition 1, we have

$$q = 2\pi/\lambda_0 = 0.001052 \text{ \AA}^{-1} \quad (9)$$

and the recoil energy equals $E_r = 0.461764 \times 10^{-9}$ eV. Thus, the recoil energy is very small compared to the resonance energy $E_r/E_0 \approx 2.2 \times 10^{-10}$.

The Debye-Waller factor can be estimated using the Debye model of isotropic crystal, which is a fair approximation also for quantum crystals such as solid helium, hydrogen or deuterium. In this model, the density of vibrational states takes the form

$$Z(w) = \begin{cases} 3w^2/w_D^3 & \text{if } w \leq w_D \\ 0 & \text{if } w > w_D, \end{cases} \quad (10)$$

in which the maximum energy of vibrations w_D is determined by the Debye temperature θ_D of the crystal: $w_D = k_B \theta_D$. The Debye temperature for solid ^4He is greater than 25 K. For the pressures 26.7–129 bar and the corresponding temperatures 1 K–4 K, which are considered in this work, $\theta_D \approx 25$ K–38 K [12] and thus $T/\theta_D \ll 1$. In the limit $T \rightarrow 0$, Eq. (4) is expressed by a simple integral. As a result, we obtain the following expression:

$$2W = \frac{3}{2} \frac{E_r}{w_D}, \quad (11)$$

which is a good approximation for $T/\theta_D \ll 1$. In the case of transition 1, one has $2W \sim 10^{-7}$. Thus, the recoil-less term in the expansion (3) is dominant and the subsequent phonon

contributions are negligible. This means that the resonance-line shift in solid helium is solely due to the collisional correction ΔE_0 . Let us note that in the case of a free $\bar{p}\text{He}^+$ atom the line shift is strictly equal to the recoil energy E_r . On the other hand, in solid helium, the recoil effect disappears since the response of the ^4He lattice to the resonance-photon absorption or emission is practically the response of a rigid lattice.

The phonon contribution to the line broadening is determined by the one-phonon term (6) with the width determined by $w_D \approx 2\text{--}3$ meV. However, this contribution can be neglected because of an extremely small amplitude of the phonon processes, which is caused by smallness of the $2W$ factor. Therefore, the collective degrees of freedom practically do not change the resonance-line width in solid ^4He . The width of the dominant recoil-less term is equal to the natural resonance width Γ_0 .

III. COLLISIONAL SHIFT OF RESONANCE LINES IN SOLID HELIUM

The collisional shift ΔE_0 of the resonance lines in crystalline ^4He is estimated here in the quasistatic limit using the method that has been discussed in detail in Ref. [1]. The line shift is expressed in terms of the pairwise potentials of $\bar{p}\text{He}^+$ interaction with a single helium atom and the pair-correlation function $g(r)$ of a condensed ^4He target for a fixed temperature and pressure. The expression $g(r)dr$ gives the probability of finding a ^4He atom in the shell $[r, r + dr]$ around a given atom. We use here the spherically symmetric pairwise potentials $V_i(r)$ and $V_f(r)$ of the $\bar{p}\text{He}^+$ -He interaction in the initial and final states of antiprotonic helium [4, 13]. As a result, the collisional contribution ΔE_0 to the resonance-line shift is approximated by the following expression:

$$\Delta E_0 = \int_0^{r_{\max}} dr g(r) \Delta V(r), \quad (12)$$

where $\Delta V(r) = V_f(r) - V_i(r)$ and r_{\max} is a cutoff. Let us note that the radius r in the function $g(r)$ denotes the distance reckoned from a given ^4He atom located in the origin. In our case, we replace this atom by the implanted antiprotonic helium atom. However, this is a reasonable approximation since the probability density calculated for the two-particle system $\bar{p}\text{He}^+ + \text{He}$ is very similar to $g(r)$ at $r \lesssim 3$ Å [1].

In the literature, the data regarding the function $g(r)$ are scarce. We use here the theoretical $g(r)$ for the solid ^4He near the melting curve at temperature $T = 1.0$ K and pressure $P = 26.7$ bar ($\rho = 190$ g/l) [14]. Also, we employ the theoretical $g(r)$ for $T = 2.5$ K at $P = 57$ bar ($\rho = 209$ g/l) and $T = 4.0$ K at $P = 129$ bar ($\rho = 234$ g/l) [15]. The functions $g(r)$ for solid and liquid ^4He are compared in Fig. 1 for $T = 1$ K and $T \approx 4$ K. Although the liquid ^4He is superfluid at 1 K and normal fluid at 4.27 K, the corresponding pair-correlation functions are very similar. Therefore, no significant change of behavior of the resonance-line shift is expected in liquid helium. On the other hand, the functions $g(r)$ for solid ^4He at the presented temperatures and densities differ significantly from each other and from the corresponding functions for liquid helium. In particular, one can see that the probability of finding a neighboring ^4He atom at $2 \text{ Å} < r < 3.5 \text{ Å}$ is much greater in the solid targets. This interval of r gives a dominant contribution to the line shift, which is shown in Fig. 2. As a result, one can expect a significant change of the line-shift behavior in solid helium.

The average number $n(r)$ of ^4He atoms,

$$n(r) = 4\pi N_0 \int_0^r dr' r'^2 g(r'), \quad (13)$$

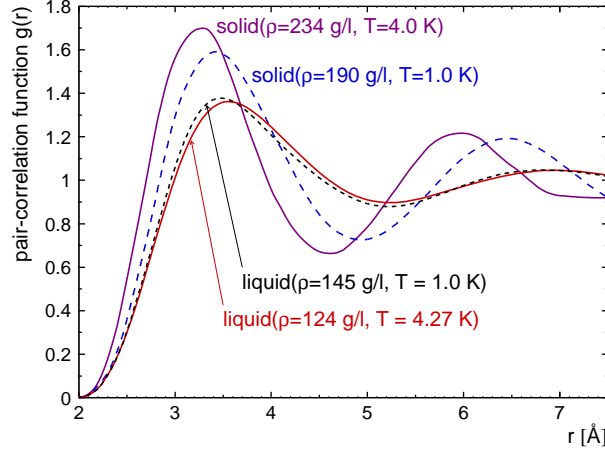


FIG. 1: (Color online) The pair-correlation functions $g(r)$ for solid [14, 15] and liquid (at the saturated-vapor pressure) [16] ^4He at several values of target density ρ and temperature T .

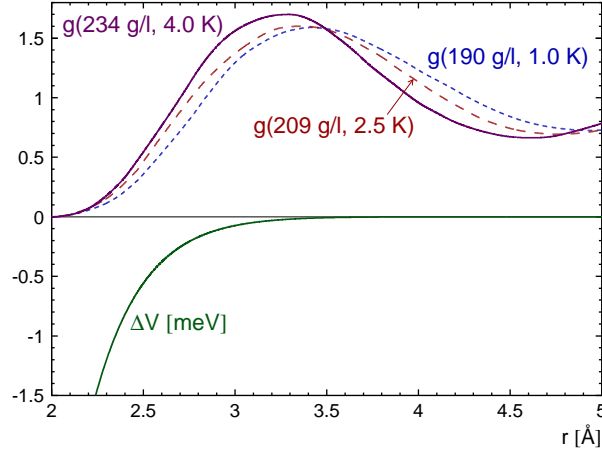


FIG. 2: (Color online) The difference $\Delta V(r)$ of the pairwise potentials $V_{(39,35)}(r)$ and $V_{(38,34)}(r)$ together with the pair-correlation functions $g(r)$ for solid ^4He [14, 15] versus the distance r between the antiprotonic helium and the ^4He atom. The densities ρ and temperatures T of the three targets are given in the plot. One can conclude from this figure that the contribution to the resonance energy shift, Eq. (12), practically comes from the interval $2.0 \text{ \AA} < r \lesssim 3.3 \text{ \AA}$, where both $\Delta V(r)$ and $g(r)$ have significant values. For $r \leq 2.0 \text{ \AA}$, the correlation function disappears due to the finite size and the short-distance repulsion of helium atoms.

which are located within the sphere of radius r around the helium atom in the origin, is shown in Fig. 3 for the three pressures. Since $n(r) < 2$ for $r \lesssim 3 \text{ \AA}$, where the absolute value of $\Delta V(r)$ has the largest amplitude, the contribution to the resonance-line shift (12) from this region is dominant. Therefore, using the pairwise interaction potentials for determination of the resonance shift in solid ^4He is a reasonable approximation.

The results of our calculations for solid ^4He for the three different target densities are summarized in Table I, where the reduced line shift $\Delta E_0/\rho$ is given in the fifth column. A dependence of the calculated reduced line shift on the upper limit r_{max} in the integral (12) is shown in Fig. 4. One can see that it is sufficient to perform integration in Eq. (12) up

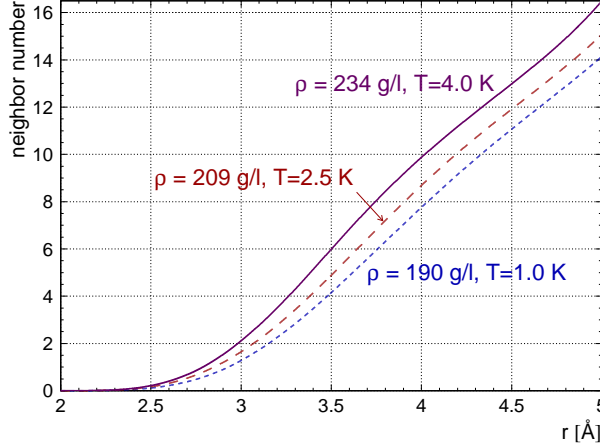


FIG. 3: (Color online) The number $n(r)$ of ^4He atoms within the sphere of radius r that surround an atom placed at $r = 0$ in solid helium.

TABLE I: The resonance-line shift ΔE_0 and the reduced line shift $\Delta E_0/\varrho$ for solid ^4He .

Temperature [K]	Pressure [bar]	Density [g/l]	ΔE_0 [GHz]	$\Delta E_0/\varrho$ [GHz l/g]
1.0	26.7	190	-99.8	-0.525
2.5	57.0	209	-130.9	-0.626
4.0	129.0	234	-164.8	-0.704

to $r_{\text{max}} \approx 3.8 \text{ \AA}$. Thus, the knowledge of the pair-correlation function above this limit is not needed. The resonance-line shifts ΔE_0 which are presented in Table I display a clear nonlinear dependence on the target density, which is in contrast to the behavior of analogous line shifts in ^4He gas [5, 6] and liquid ^4He above $T = 2.17 \text{ K}$ [1]. The absolute values of the reduced line shifts in solid helium are greater than the values of the corresponding line shifts in liquid ^4He (e.g., $\Delta E_0/\varrho = -0.427 \text{ GHz l/g}$ for $\varrho = 146 \text{ g/l}$ at $T = 2.27 \text{ K}$ [1]).

IV. CONCLUSIONS

The experimental and theoretical investigation of the density dependence of the resonance-line shifts in gaseous helium and the projects of the ASACUSA Collaboration at CERN for the high-accuracy laser spectroscopy of $\bar{p}\text{He}^+$ atoms in liquid ^4He has motivated the present work. In particular, we have studied the influence of collective degrees of freedom in solid ^4He on the broadening and shift of the resonance lines of antiprotonic helium located in this target.

We have found that the resonant absorption or emission of a laser photon by the $\bar{p}\text{He}^+$ atom implanted in solid ^4He is a fully recoil-less process which takes place in the rigid lattice and thus is analogous the Mössbauer effect. This is due to a very small momentum transfer to the lattice of about 0.001 \AA^{-1} and extremely small amplitudes of phonon processes, which are simultaneous with the resonant transition in the antiprotonic helium. Therefore, there is

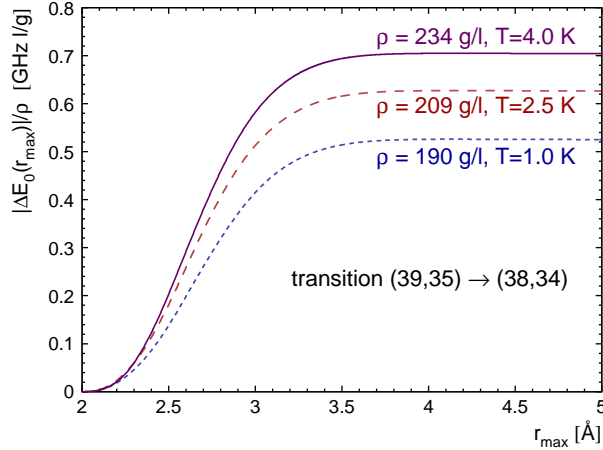


FIG. 4: (Color online) The absolute value $|\Delta E_0|/\rho$ of the reduced resonance-line shift in solid ^4He as a function of r_{max} .

exactly no contribution to the resonance-line shifts from the collective motion in solid helium. On the other hand, the resonance lines in the case of $\bar{p}\text{He}^+$ atom in a dilute helium gas are shifted by the corresponding recoil energy, which is however very small. The broadening of resonance-line shifts due to the collective motion in crystalline ^4He is determined by the one-phonon processes and equals about 2-3 meV, which is a typical maximum phonon energy in solid helium. However, the amplitude of such processes is smaller by many orders of magnitude than the recoil-less process so that this broadening cannot be observed in experiments. As a result, the total broadening and shift of the resonance lines in solid helium are determined by the collisional effects. The magnitude of the reduced collisional shift $\Delta E_0/\rho$ for the resonance transition $(39,35) \rightarrow (38,34)$, which has been calculated in the quasistatic approach, ranges from -0.525 to -0.704 GHz l/g when the density of solid ^4He varies from 190 to 234 g/l. Therefore, the density dependence of the total line shift is clearly nonlinear, which is in contrast to the behavior of the analogous line shifts in gaseous and normal liquid ^4He .

In order to improve the accuracy of the presented evaluation of the collisional contribution to the resonance-line shifts it is indispensable to calculate the potentials of $\bar{p}\text{He}^+$ interaction with at least two helium atoms. Also, this would enable a reliable estimation of the collisional broadening of the spectral lines. However, a calculation of the appropriate potentials is much more complicated than in the case of one neighboring He atom.

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